

1,4-Benzoquinone
106-51-4 | DTXSID6020145

Model Performance

Model

Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.87	0.81	0.87	0.82	0.86	0.86

Model Results

Predicted value: 3.41e-01 mol/L

Global applicability domain: Inside

Local applicability domain index: 6.02e-01

Confidence level: 5.08e-01

Nearest Neighbors from the Training Set

Image not found

p-Benzoquinone monoxime

Measured: 2.84e-02

Predicted: 4.68e-02

Image not found

1-Methyl-2-oxocyclopentane-1-carbonitrile

Measured: 8.12

Predicted: 2.07

Image not found

2,4-Pentanedione

Measured: 1.66

Predicted: 1.64

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5,5-Dimethyl-1,3-cyclohexanedione

Measured: 2.97e-02

Predicted: 9.52e-02